Decay on several sorts of heterogeneous centers: Special monodisperse approximation in the situation of strong unsymmetry. 4. Numerical results for the approximation of essential asymptotes

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This manuscript directly continues [1], [2], [3]. All definitions and formulas have to be taken from [1]. The numerical results for comparison with the total monodisperse approximation has to be taken from [2]. The numerical results for the floating monodisperse approximation can be taken from [3].

1 Calculations

We have to recall again the system of the condensation equations. It can be written in the following form

$$G = \int_0^z \exp(-G(x))\theta_1(x)(z-x)^3 dx$$

$$\theta_1 = exp(-b \int_0^z \exp(-G(x))dx)$$

with a positive parameter b and have to estimate the error in

$$N = \int_0^\infty \exp(-lG(x))dx$$

with some parameter l.

We shall solve this problem numerically and compare our result with the already formulated models. In the model of the total monodisperse approximation we get

$$N_A = \int_0^\infty \exp(-lG_A(x))dx$$

where G_A is

$$G_A = \frac{1}{b}(1 - \exp(-bD))x^3$$

and the constant D is given by

$$D = \int_0^\infty \exp(-x^4/4)dx = 1.28$$

Numerical results are shown in [2].

In the model of the floating monodisperse approximation we have to calculate the integral

$$N_B = \int_0^\infty \exp(-lG_B(x))dx$$

where G_B is

$$G_B = \frac{1}{b}(1 - \exp(-b\int_0^{z/4} \exp(-x^4/4)dx))z^3$$

$$G_B \approx \frac{1}{b}(1 - \exp(-b(\Theta(D - z/4)z/4 + \Theta(z/4 - D)D)))z^3$$

Numerical results are shown in [3].

It is very attractive to spread the approximation for the last integral at small z for all z (as it was done in the intermediate situation in [4] when we solved the algebraic equation on the parameters of the spectrum (in the intermediate situation it is absolutely justified). Then we came to the third approximation

$$N_C = \int_0^\infty \exp(-lG_C(x))dx$$

where G_C is

$$G_C \approx \frac{1}{b}(1 - \exp(-bz/4))z^3$$

This approximation will be called as "approximation of essential asymptotes". The real advantage of this approximation is the absence of the exponential nonlinearity. When this approximation will be introduced into

equation on the parameters of the condensation process there will be no numerical difficulties to solve it.

We have tried all mentioned approximations for b from 0.2 up to 5.2 with the step 0.2 and for l from 0.2 up to 5.2 with a step 0.2. We calculate the relative error in N. The results are drawn in fig.1 for N_C where the relative errors are marked by r_3.

We see that the relative errors of N_B and N_C are very small and practically the same. One can not find the difference between fig.1 in [3] and fig.1 here.

The maximum of errors in N_B and N_C lies near $l = 0$. So, we have to analyse the situation with small values of l. It was done in fig.2 for N_C. We see that we can not find the maximum error because it increases at small b. Then we have to calculate the situation with $b = 0$. Here we have to solve the following equation

$$G = \int_0^\infty \exp(-G(x))(z - x)^3 dx$$

and to compare

$$N = \int_0^\infty \exp(-lG) dx$$

with

$$N_A = \int_0^\infty \exp(-lDz^3) dz$$

$$N_B = \int_0^\infty \exp(-l(\Theta(z/4 - D)Dz^3 + \Theta(D - z/4)z^4/4)) dz$$

$$N_C = \int_0^\infty \exp(-lz^4/4) dz$$

We can not put here $l = 0$ directly.

The results are shown in fig.3. One can see one curve with two wings. The upper wing corresponds to the error of N_A and the lower corresponds to the relative error in N_B and N_C. At $l = 0$ these wings come together. We see that our hypothesis (the worst situation for the floating monodisperse approximation takes place when the first type heterogeneous centers are unexhausted) is really true.

The worst situation is when b is near zero and l lies also near zero. Here we can use the total monodisperse approximation to estimate the error. It is clear that the relative error in N_A is greater than in N_B (not in N_C). So, we can calculate r_1, see that when b goes to zero it decreases (it is clear also

from the physical reasons) and estimate the error r_2 at $b = 0$, $l = 0$ by R_1 calculated at small b and $l = 0$. Then one can see that it is small.

An interesting problem is to see whether N_B and N_C are different or no. Earlier we can not see the difference. In fig.4 one can see the ratio r_2/r_3 plotted at $b = 0$ and can note that only for $l \approx 0.01 \div 0.02$ one can see the small difference. It means that to see the difference between these approximations the ratio between the scale of the first type centers nucleation and the scale of the second type centers nucleation must be giant. Even at giant values the difference is small.

References

[1] V. Kurasov, Preprint cond-mat@xxx.lanl.gov get 0001104

[2] V. Kurasov, Preprint cond-mat@xxx.lanl.gov get 0001108

[3] V. Kurasov, Preprint cond-mat@xxx.lanl.gov get 0001112

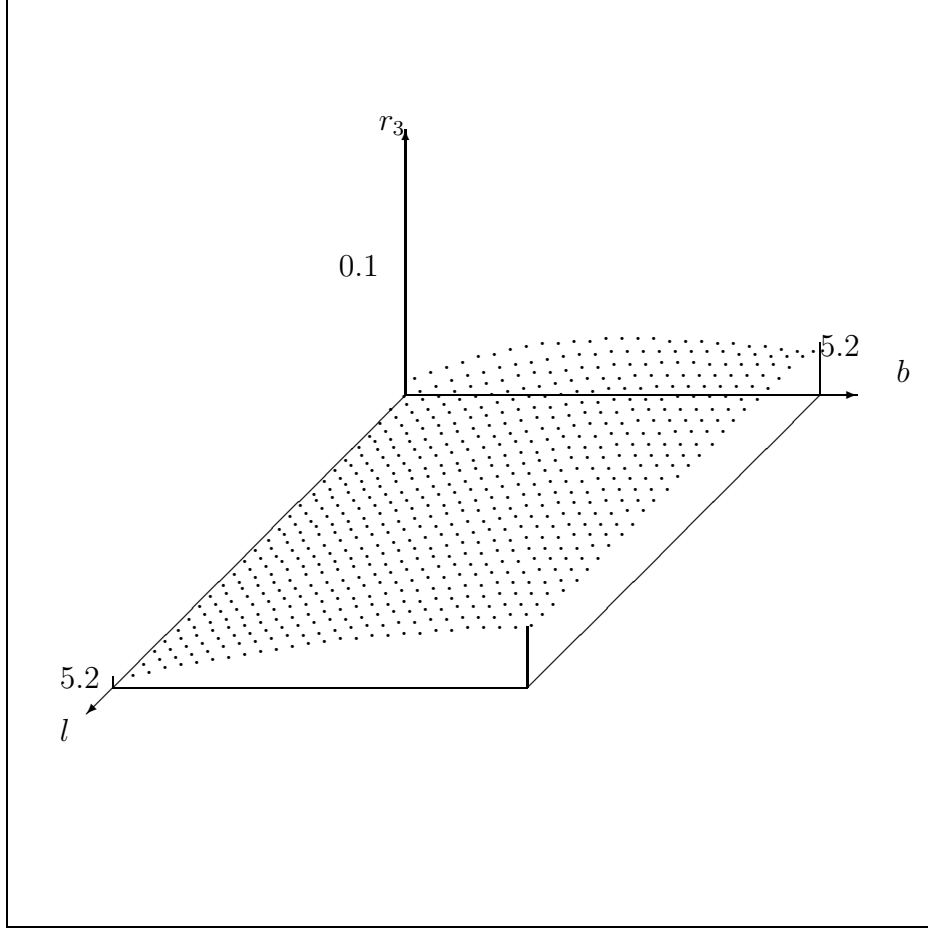[4] V.B.Kurasov, Deponed in VINITI 2594B95 from 19.09.1995, 28 p.

Fig.1

The relative error of N_C drawn as the function of l and b. Parameter l goes from 0.2 up to 5.2 with a step 0.2. Parameter b goes from 0.2 up to 5.2 with a step 0.2.

One can see the maximum at small l and moderate b. One can not separate N_B and N_C according to fig.1 in [3] and fig.1.
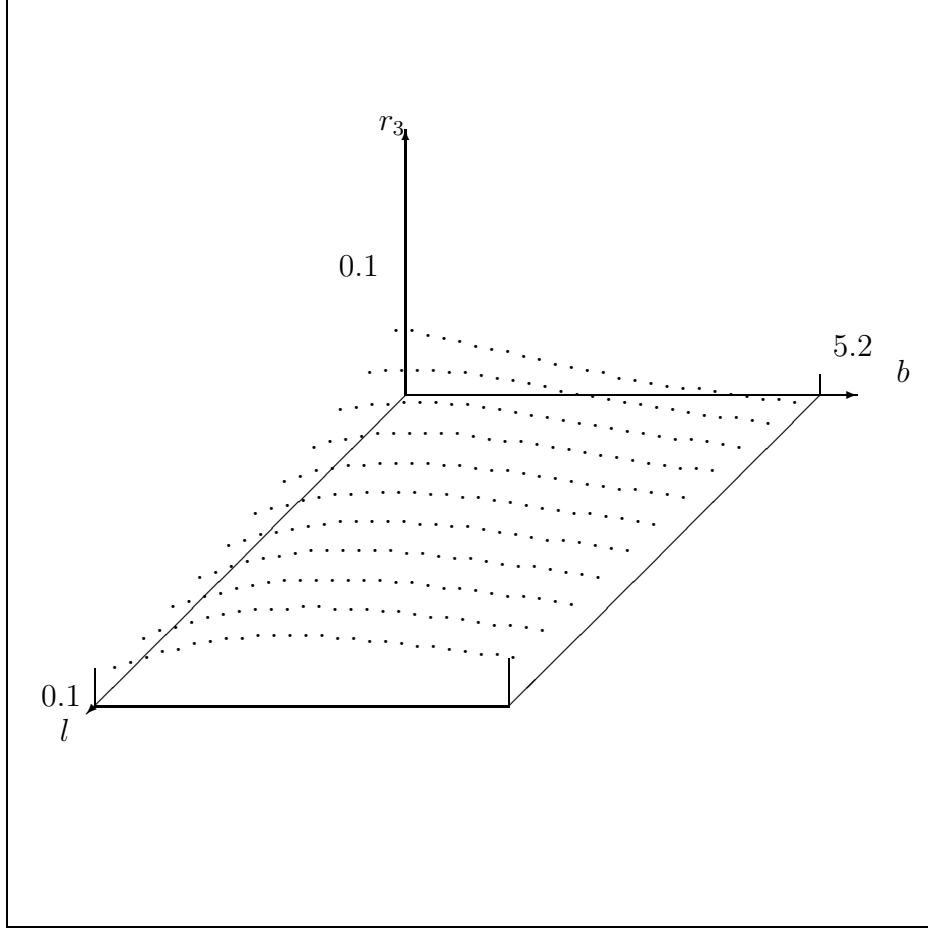
Fig.2

The relative error of N_C drawn as the function of l and b. Parameter l goes from 0.01 up to 0.11 with a step 0.01. Parameter b goes from 0.2 up to 5.2 with a step 0.2.

One can see the maximum at small l and small b. One can note that now the values of b corresponding to maximum of the relative errors become small. One can not separate N_B and N_C according to fig.2 in [3] and fig.2 here.
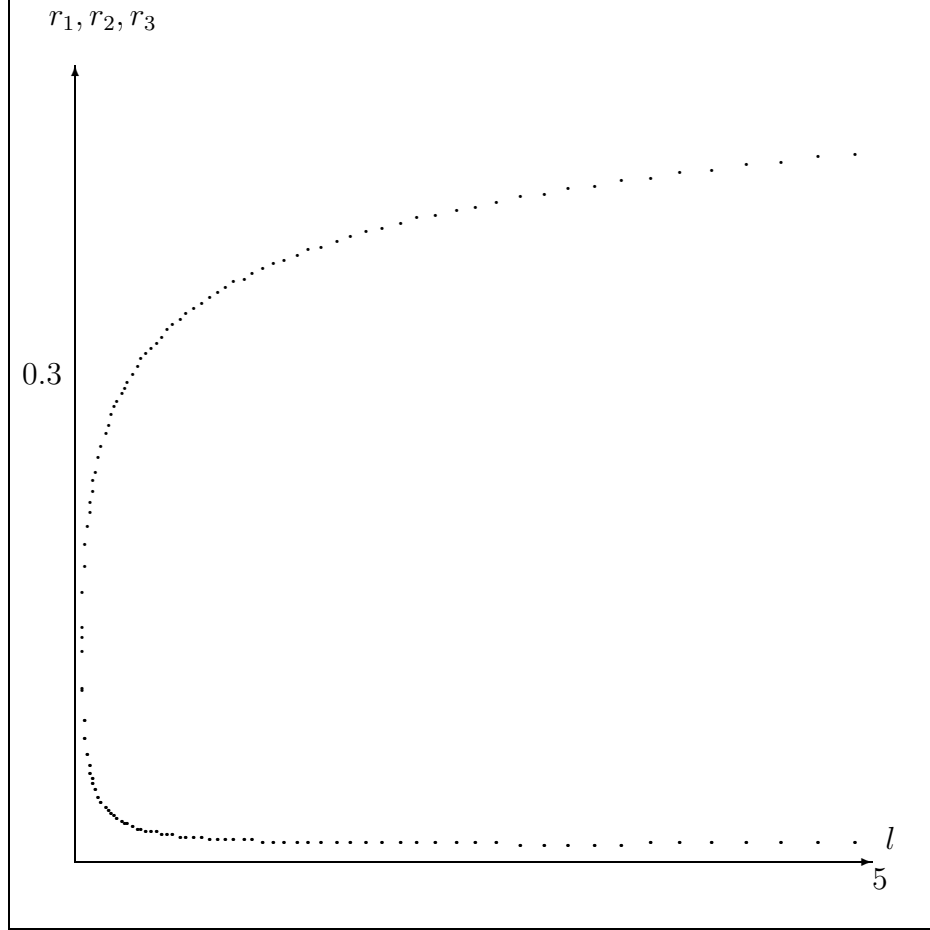
Fig.3

The relative errors of N_A, N_B and N_C drawn as the function of l at $b = 0$. Parameter l goes from 0.01 up to 5.01.

One can see two wings which come together for b near 0. The upper wing corresponds to the relative error of N_A. The lower wing corresponds to the relative errors of N_B and N_C. One can not separate them.

One can see that r_1 decreases when b goes to 0 and can estimate r_2 by r_1 at small l.
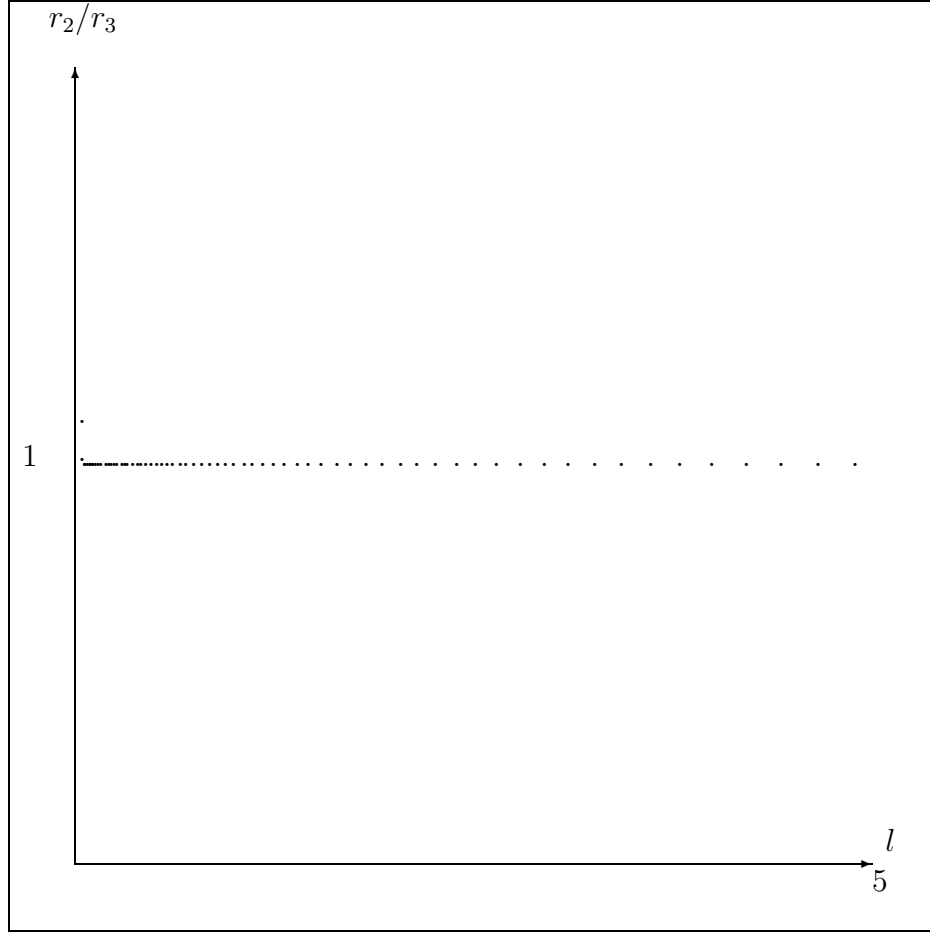
Fig.4

The ratio r_2/r_3 drawn as the function of l at $b = 0$. Parameter l goes from 0.01 up to 5.01.

One can see the difference between r_2 and r_3 only at very small values of b (only the first two points corresponding to $l = 0.01$ and $l = 0.02$). So, N_3 can be also considered as a suitable approximation.